

Reentrant BCS-BEC crossover and a superfluid-insulator transition in optical lattices

Zhaochuan Shen, L. Radzihovsky, V. Gurarie

Department of Physics, University of Colorado, Boulder, CO 80309, USA

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We study thermodynamics of a two-species Feshbach-resonant atomic Fermi gas in a periodic potential, focusing in a deep optical potential where a tight binding model is applicable. We show that for more than half-filled band the gas exhibits a reentrant crossover with decreased detuning (increased attractive interaction), from a paired BCS superfluid to a Bose-Einstein condensate (BEC) of molecules of holes, back to the BCS superfluid, and finally to a conventional BEC of diatomic molecules. This behavior is associated with the non-monotonic dependence of the chemical potential on detuning and the concomitant Cooper-pair/molecular size, larger in the BCS and smaller in the BEC regimes. For a single filled band we find a quantum phase transition from a band insulator to a BCS-BEC superfluid, and map out the corresponding phase diagram.

Feshbach resonances have become an essential experimental tool in the exploration of interacting degenerate atomic gases, allowing, for a realization of Fermi superfluidity tunable from a weakly-paired BCS to a strongly-paired molecular regime[1–6].

Confinement of atomic gases in optical lattices is another powerful technique for realizing and tuning strong correlations[7], allowing experimental investigation of a variety of lattice quantum many-body phenomena, such as the superfluid to Mott insulator transition[8].

Naturally, recent attention has focused on the rich combination of Feshbach-resonant gases in optical lattices[9–11]. Although considerable progress has recently been made[12–18], a general theoretical description of such system is challenging even at the two-body level as it involves a projection of the Feshbach resonance physics onto the eigenstates of the periodic potential. Optical lattice shifts bulk Feshbach resonances and induces new ones.

Yet it is possible to argue[19, 20] that in a sufficiently deep optical lattice (bandwidth much smaller than a bandgap), even in the vicinity of a broad Feshbach resonance, the single band tight binding model with on-site attraction (attractive Hubbard model) $U(a)$, a function of a vacuum scattering length a is sufficient to describe the physics. Likewise, for a narrow Feshbach resonance in a deep lattice a tight binding model of open-channel fermions and closed-channel bosonic molecules coupled by an on-site interconversion term, Eq. (1) is appropriate.

In this Letter, focusing on the deep lattice regime we establish that for a broad resonance, a two-component Fermi gas above half filling undergoes a BCS-BEC crossover with the molecular condensate in the BEC regime composed of holes; below half filling the crossover is to a conventional condensate of diatomic molecules. The BCS and BEC regimes are separated by an analog of a unitary point where the thermodynamic properties of the gas are given by a universal function of the band filling fraction. For a narrow resonance [4, 21], while below half filling the behavior is qualitatively equivalent

to its broad-resonance counterpart, above half filling the crossover is non-monotonic and reentrant. Upon decreasing the detuning the phenomenology crosses over from a BCS regime to a BEC regime of molecules composed of holes, back to a BCS regime and finally to a BEC regime of diatomic molecules. This rich behavior, illustrated in Fig. (1a) is associated with a corresponding non-monotonic dependence of the chemical potential on the Feshbach resonance detuning. Concomitantly, the size of a Cooper pair/molecule changes non-monotonically, with the BCS and BEC regimes respectively characterized by large and small pair sizes in units of the interatomic spacing. This resonant lattice phenomenology can in principle be probed by measuring correlations in the gas after its free expansion[22, 23], through RF spectroscopy[24], compressibility, and via details of the atomic cloud's density profile[7], as illustrated in Fig. 2.

Finally, we find that for a narrow resonance, a fully filled lattice (band filling of 2) exhibits a quantum phase transition between a band insulator and a paired superfluid, absent for a broad resonance or in the absence of an optical lattice. This latter transition can be best detected in the “wedding cake” density profile, a layered structure of the gas when placed in an overall confining harmonic potential, with a shell of a band insulator sandwiched by an inner superfluid core and an outer superfluid shell.

We now outline the derivation of these predictions. We study fermionic atoms in an optical lattice which contains N sites and M atoms (atom filling fraction $n = M/N$) for both the one- and two-channel models. The starting point is to consider the tight-binding two-channel Hamiltonian

$$H = -t \sum_{\langle \mathbf{r}, \mathbf{r}' \rangle, \sigma} c_{\mathbf{r}, \sigma}^\dagger c_{\mathbf{r}', \sigma} - \mu \sum_{\mathbf{r}, \sigma} c_{\mathbf{r}, \sigma}^\dagger c_{\mathbf{r}, \sigma} - t_b \sum_{\langle \mathbf{r}, \mathbf{r}' \rangle} b_{\mathbf{r}}^\dagger b_{\mathbf{r}'} + (\nu_0 - 2\mu) \sum_{\mathbf{r}} b_{\mathbf{r}}^\dagger b_{\mathbf{r}} + g \sum_{\mathbf{r}} (b_{\mathbf{r}}^\dagger c_{\mathbf{r}, \uparrow} c_{\mathbf{r}, \downarrow} + h.c.). \quad (1)$$

Here, $c_{\mathbf{r}, \sigma}^\dagger$, $c_{\mathbf{r}, \sigma}$ are the creation and annihilation operators of the fermionic atoms at lattice site \mathbf{r} with spin σ , $b_{\mathbf{r}}^\dagger$, $b_{\mathbf{r}}$ are creation and annihilation operators of bosonic closed-channel molecules, μ is the chemical potential, g is

the coupling, ν_0 is the “bare” detuning, t (t_b) is the hopping matrix element for the atoms (molecules) and $\langle \mathbf{r}, \mathbf{r}' \rangle$ denotes pairs of nearest neighbor sites. In the absence of interactions, the bosons and fermions are free particles, with the tight-binding dispersion of atoms given by

$$\epsilon_{\mathbf{k}} = -2t(\cos k_x + \cos k_y + \cos k_z), \quad \xi_{\mathbf{k}} = \epsilon_{\mathbf{k}} - \mu, \quad (2)$$

where the lattice constant is taken to be 1. Considerable progress in understanding the thermodynamics can be obtained through a mean-field approximation where closed-channel molecular field is replaced by a classical field:

$$b_{\mathbf{q}} \approx B \delta_{\mathbf{q},0}, \quad (3)$$

with $b_{\mathbf{q}}$ a Fourier transform of $b_{\mathbf{r}}$. Diagonalizing the resulting quadratic Hamiltonian and varying corresponding ground state energy with respect to μ and B^* gives the number and gap equations:

$$n = \int_{BZ} \frac{d^3k}{(2\pi)^3} \left(1 - \frac{\xi_k}{\sqrt{\xi_k^2 + g^2 |B|^2}} \right) + 2|B|^2, \quad (4)$$

$$\nu_0 - 2\mu = \frac{g^2}{2} \int_{BZ} \frac{d^3k}{(2\pi)^3} \frac{1}{\sqrt{\xi_k^2 + g^2 |B|^2}}, \quad (5)$$

with the integrals over the entire Brillouin zone (BZ). The solutions give μ and $|B|$ as a function of detuning ν_0 .

We first analyze these equations in a limit of a broad resonance, corresponding to taking ν_0 and g to infinity, while keeping their ratio $U = g^2/\nu_0$ finite. In this limit, the closed-channel molecules $b_{\mathbf{q}}$ can be adiabatically eliminated (integrated out) reducing the Hamiltonian Eq. (1) to that of an attractive Hubbard model with the interaction strength U .

In this limit the Eqs. (4) and (5) become

$$n = \int_{BZ} \frac{d^3k}{(2\pi)^3} \left(1 - \frac{\xi_k}{\sqrt{\xi_k^2 + \Delta^2}} \right), \quad (6)$$

$$\frac{1}{U} = \frac{1}{2} \int_{BZ} \frac{d^3k}{(2\pi)^3} \frac{1}{\sqrt{\xi_k^2 + \Delta^2}}, \quad (7)$$

where $\Delta = g|B|$ is finite, while $|B|$ goes to zero in the broad resonance limit.

An important feature of these equations (by particle-hole symmetry that holds even beyond the mean-field approximation [25]) is that the sign of the chemical potential μ depends on whether the band filling fraction n is above or below 1 (corresponding to above or below half filling), with $\mu = 0$ for $n = 1$ independent of Δ and U . Mathematically, the latter is captured by $\int d^3k \xi_k F(|\xi_k|) = 0$ for any function $F(|\xi_k|)$ for $\mu = 0$. To see that the sign of μ is independent of Δ and therefore U , suppose $n > 1$. Then for $\Delta = 0$ (corresponding

to $U \rightarrow 0$), the right hand side of Eq. (6) reduces to the Fermi-Dirac step-function, obviously giving $\mu > 0$. Now, for a nonzero Δ , μ must remain positive since μ crossing zero at any Δ would imply $n = 1$, contradicting the $n > 1$ assumption. Similarly, if $n < 1$, then $\mu < 0$, independent of U .

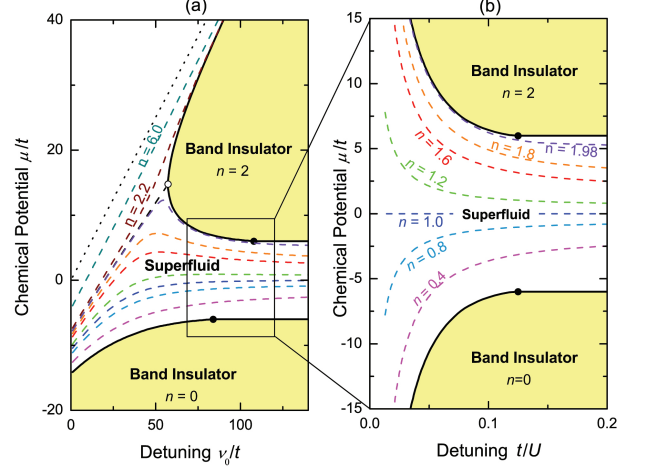


FIG. 1: The normalized chemical potential in, two-channel model (a) (for $g/t = 20\sqrt{2}$) and one-channel model (b). Colored dashed lines correspond to different density n of the gas. The leftmost dashed line in (a) has $n > 2$. The dots on black lines correspond to the threshold of the molecule formation in the vacuum.

Solving Eqs. (6,7) numerically gives the relation between μ and U shown in Fig. (1b). We thus observe that in this broad resonance regime, for $n < 1$ the system undergoes a conventional BCS-BEC crossover, reaching the BEC regime for strong attractive interaction U (or equivalently for reduced detuning ν_0), where large negative chemical potential gives (negative) half the binding energy of molecules formed by pairs of fermionic atoms. In contrast, for $n > 1$, as a reflection of particle-hole mapping between $n < 1$ and $n > 1$ fillings, the $\mu > 0$ chemical potential actually grows with increased attractive interaction, crossing above the top of the band for large attractive U . This corresponds to a BCS-BEC crossover to a BEC of molecules of two holes in the Fermi sea with the chemical potential tracking half of their binding energy. At exactly half filling ($n = 1$) there is no BCS-BEC crossover, with chemical potential remaining pinned exactly at $\mu = 0$ for all U , consistent with particle-hole symmetry of the Hubbard model at half-filling.

At $n = 0$ and $n = 2$ the Eqs. (6,7) can be straightforwardly solved analytically. For example, at $n = 0$ we expect that $\Delta = 0$ and $\mu \leq -6t$, dropping below the bottom of the band. Then Eq. (6) is automatically satisfied

($\xi_{\mathbf{k}} > 0$ for all \mathbf{k}), and Eq. (7) reduces to

$$\frac{1}{U} - \frac{C}{4t} = \frac{1}{2} \int_{BZ} \frac{d^3k}{(2\pi)^3} \left[\frac{1}{\xi_{\mathbf{k}}} - \frac{1}{\epsilon_{\mathbf{k}} + 6t} \right], \quad (8)$$

where $C = \int_{BZ} \frac{d^3k}{(2\pi)^3} \frac{1}{3 - \cos(k_x) - \cos(k_y) - \cos(k_z)} \approx 0.505$. Writing the right hand side of the gap equation in this form allows us to expand the cosines around $\mathbf{k} = 0$ and extend the integral to infinity (valid as long as $-\mu/(6t) - 1 \ll 1$) to find

$$\frac{1}{U} - \frac{C}{4t} = -\frac{\sqrt{|\mu| - 6t}}{8\pi t^{3/2}}. \quad (9)$$

This is the $\mu(U)$ relation at the lowest density, $n = 0$, corresponding to half of the binding energy of the zero momentum molecule formed by two atoms. In order for the molecule to form in 3D, U must exceed a threshold attraction, $U > 4t/C$, as is known in the absence of lattice potential[4, 26]. We note, however, that at a finite center of mass momentum at the Brillouin Zone boundary, a molecule can form at an arbitrarily weak attraction even in 3D[18].

Similarly by particle-hole symmetry, at $n = 2$ close to the top of the band $\mu(U)$ is also given by Eq. (9). The full $\mu(U, n)$ dependence for $0 < n < 2$ can be obtained through a straightforward numerical or an approximate analytical analysis of Eqs. (6, 7). However, it should be kept in mind that these are in themselves only valid within a mean field approximation, except at very small or very large U (at $n \neq 1$).

We observe that at a special value $U = 4t/C$ the interaction strength drops out of Eqs. (6, 7), corresponding to a divergent scattering length, just like at the unitary point of the BCS-BEC crossover in the absence of a lattice potential. Although these mean-field equations are approximate, this general feature holds more generally, with the chemical potential at a unitary point $U = U_*$ given by a universal function of particle density

$$\mu/t = f(n). \quad (10)$$

with the property $f(2 - n) = -f(n)$ dictated by the particle-hole symmetry. In the dilute $n \rightarrow 0$ limit, we recover the lattice-free result

$$f(n) \approx -6 + \xi (3\pi^2 n)^{2/3}, \quad (11)$$

where ξ is the Bertsch parameter[27], $\xi \approx 0.4$ [28–30]. The full function $f(n)$ is not known but can be computed numerically.

In contrast to the above broad resonance limit (one-channel model), where n is restricted to $0 \leq n \leq 2$, in the two-channel model, Eq. (4) the filling fraction is no longer limited by two particles per site, as closed-channel bosonic states can accommodate an arbitrary number of fermionic atom pairs even if all states in the fermionic

band are occupied. We next study the ground state behavior of the two-channel model encoded in Eqs. (4,5), that in the narrow resonance limit, $g\sqrt{n} \ll E_F$ are quantitatively trustworthy across the entire phase diagram and in the opposite broad resonance limit reduce to those of the one-channel model discussed above.

Solving these equations numerically leads to the $\mu - \nu_0$ phase diagram illustrated in Fig. (1a). Its many features can be understood analytically, particularly for a narrow resonance. It displays a band insulator (BI) and a paired superfluid (SF) phases, depending on the range of the chemical potential and detuning. For large positive detuning ν_0 , closed-channel molecules are separated by a large gap above the fermionic band, leading to a weak attractive interaction for the atoms. Thus, for a partially filled fermionic band, $0 < n < 2$, the chemical potential $\mu(n)$ sits within the band $-6t < \mu < 6t$, and the ground state is a weakly-paired BCS superfluid. Increasing the filling to $n = 2^-$ pushes the chemical potential to the top of the band, $\mu(2^-) = 6t$. Since the fermionic band is then full at $n = 2$, a further increase in n can only be accommodated by populating the closed-channel molecular state. For large ν_0 , the chemical potential therefore jumps from $\mu(2^-) = 6t$ to $\mu(2^+) \approx \nu_0/2$, which thus determines the lower and upper phase boundaries of the $n = 2$ BI.

Reducing the detuning ν_0 brings down the molecular state and leads to its hybridization with the pairs of the fermionic band states and a concomitant increase in the attractive interactions. Below half-filling, $n < 1$ this leads to a monotonic emptying of the fermionic band as the BCS superfluid crosses over to the molecular BEC, familiar from a narrow resonance BCS-BEC crossover in the absence of the periodic potential[4].

The phase boundary between the paired superfluid and $n = 0$ BI (vacuum) can then be found exactly, as it corresponds to a limit of a two-atom ground state, with $\mu_c(\nu_0) \equiv \mu(\nu_0, n = 0, B = 0)$. While for large positive ν_0 , the phase boundary $\mu_c(\nu_0) = -6t$ follows the bottom of the band, for $\nu_0 < \nu_0^*$, a true stable molecular bound state (not just a resonance) peels off from the bottom of the band following half of the molecular binding energy. To see this emerge from Eqs. (4,5), we set $n = 0$, $B = 0$ and note that for $\mu \leq -6t$ (below the bottom of the band) the number equation, Eq. (4) is automatically satisfied. The gap equation then gives

$$\nu_0 = \frac{g^2}{4t} C + 2\mu - g^2 \frac{\sqrt{|\mu| - 6t}}{8\pi t^{3/2}}. \quad (12)$$

For detuning just below $\nu_0^* = g^2 C / (4t) - 12t$ the dependence is quadratic $\mu_c(\nu_0) + 6t \sim -(\nu_0^* - \nu_0)^2$ and crosses over to linear behavior $\mu_c(\nu_0) \sim \frac{1}{2}(\nu_0 - \nu_0^*)$, following the closed-channel level, as expected from the lattice-free analysis[4].

Similar to broad resonance, Eq. (12) also depicts the phase boundary of $n = 2$. On this boundary the

threshold value of detuning below which the molecular bound state of two holes can first appear is given by $\nu_0^* = g^2 C / (4t) + 12t$, with $\mu_c = 6t$, indicated by a dot in Fig. (1a). Near and below this threshold point, $\sqrt{\mu - 6t}$ dominates and leads to a lower branch that grows quadratically, corresponding to half the binding energy of two holes. This reflects the particle-hole symmetry near this point and is consistent with earlier analysis of the broad resonance limit. The upper branch anticipated on general grounds, at large positive detuning asymptotes to the linearly growing solution, $\mu_c(\nu_0) \sim \nu_0/2$, corresponding to the nearly decoupled closed-channel state that forms the upper phase boundary of the $n = 2$ BI.

From further analysis of Eqs. (4,5), for $n \neq 2$ we find the ground state is a superfluid for all ν_0 , with the chemical potential $\mu(n, \nu_0)$ a smooth function of the filling n and detuning ν_0 (i.e., exhibits a finite superfluid compressibility), as indicated by dashed curves in Fig. (1a). For $1 < n < 2$, $\mu(n, \nu_0)$ displays a non-monotonic dependence with ν_0 , that leads to a reentrant BCS-BEC crossover of holes at intermediate detuning and a conventional one of atoms at large negative detuning.

In contrast, at $n = 2$ the system undergoes a quantum phase transition, shown on Fig. (2a), from a band insulator to a paired-hole superfluid as ν_0 is lowered below a critical value $\nu_c = \nu_0^* - \frac{g^4}{512\pi^2 t^3}$ corresponding to the tip of the band insulator lobe at $\mu_c \equiv \mu(2, \nu_c) = 6t + \frac{g^4}{1024\pi^2 t^3}$ in Fig. (1a).

The onset of superfluid order close ν_c , where B is small, can be studied analytically by expanding the number and gap equations, Eqs. (4,5) in Taylor series in $|B|^2$. This gives that inside the SF phase below ν_c at $n = 2$, $\mu(2, \nu_0)/t$ is a line of slope $3/4$. Around the critical point, the superfluid order parameter displays the standard mean-field onset, $B \sim (\nu_c - \nu_0)^{1/2}$. The paired condensate (encoded in closed-channel molecular) density $|B|^2$ as a function of detuning, for different atom densities n is illustrated in Fig. (2a), clearly revealing the BI-SF at $n = 2$.

Because the fermionic $n=2$ BI is continuously connected to a bosonic Mott insulator at filling of one boson per site, beyond mean-field theory (valid for narrow resonance) we expect this particle-hole symmetric transition to be in the $d+1$ dimensional xy universality class. Among a variety of other probes, such as thermodynamics, density profile, time of flight, and noise, the BI-SF transition can be detected via compressibility, which enters the speed of sound for the superfluid mode, that we show vanishes at the critical point and grows as $(n - 2)^{2/3}$ away from it[20].

To make contact with cold-atoms experiments, the trap potential $V(r)$ must be incorporated. This can be straightforwardly done through the local density approximation, $\mu \rightarrow \mu_{\text{local}}(r) = \mu - V(r)$, where the local chem-

ical potential $\mu_{\text{local}}(r, N, \nu_0)$ is maximum in the center of the cloud and drops off at its edges, and the global $\mu(N, \nu_0)$ is set by the total number of atoms N in the gas. The resulting radial density profile $\rho(r)$ is simply determined by a cut through the bulk phase diagram in Fig. (1a) with $\rho(r) = n(\mu_{\text{local}}(r, N, \nu_0))$. For $\nu_0 > \nu_c$ and average filling above 2 this predicts an $n > 2$ superfluid core, surrounded by a shell of an $n = 2$ band insulator (with requisite “wedding cake” plateau), that is further surrounded by a superfluid at $n < 2$. This is shown in Fig. (2b) for different detunings.

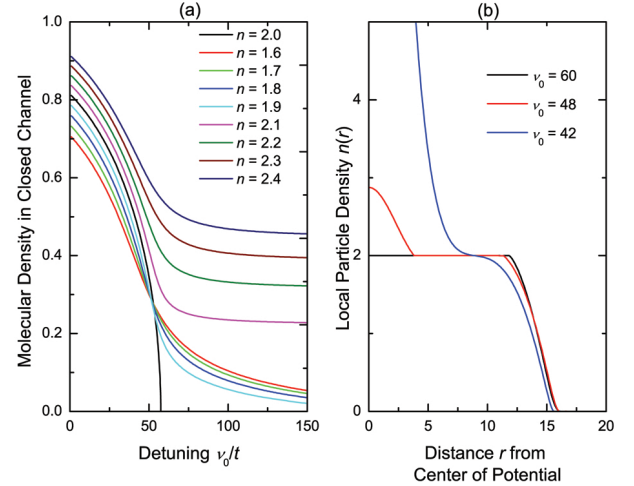


FIG. 2: (a) Paired condensate (closed-channel molecular) density $|B|^2$ as a function of detuning at different total atom densities n . At total density $n = 2$, the molecular density vanishes above certain critical detuning, signaling a quantum phase transition into a band insulator. (b) Radial atomic density $\rho(r)$ of a trapped gas in the local density approximation. The plateau corresponds to an $n = 2$ band insulator shell, sandwiched by an inner ($n > 2$) and outer ($n < 2$) superfluids.

To summarize, we studied an s-wave Feshbach resonant Fermi gas in a deep lattice potential faithfully modeled by a single band two-channel model. We showed that for above half lattice filling it exhibits an interesting reentrant BCS-BEC crossover phenomenology of paired holes and atoms associated with the nonmonotonic dependence of the chemical potential on detuning. For a single filled band we find a quantum phase transition from an $n = 2$ band insulator to a BCS-BEC superfluid, and map out the corresponding phase diagram. We expect that these predictions should be testable with current state of the art experiments on Feshbach-resonant Fermi gases in optical lattices.

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